

Thermodynamic Calculations of Hydrogen-Oxygen Detonation Parameters for Various Initial Pressures

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Composition, temperature, pressure and density behind a stable detonation wave and its propagation rate have been calculated for seven hydrogen-oxygen mixtures at 1, 5, 25 and 100 atm initial pressure, and at an initial temperature of 40 C. For stoichiometric mixtures the calculations also include an initial temperature of 200 C. According to these calculations the detonation velocities of hydrogen-oxygen mixtures increase with increasing initial pressure, but decrease slightly when the initial temperature is raised from 40 to 200 C. The calculated detonation velocities agree satisfactorily with values determined experimentally. These values will be published in the near future.

THE CALCULATIONS are based on the assumption that complete thermodynamic and chemical equilibrium is established in the wave. Dissipating effects such as viscosity, heat transfer by conduction and radiation, and chemical reaction rate phenomena are disregarded. The calculations were carried out for hydrogen-oxygen mixtures using a rigorous method developed by Edse (1).³ Other gaseous reactants will be treated in a future paper.

The detonation parameters are derived from the Hugoniot equation for the reacted gas mixture in equilibrium, and from the condition that the detonation velocity is the minimum wave velocity of the possible velocities for the given state of the combustible gas. Thus the results are based

on the Chapman-Jouguet point at which the velocity of the reacted gas relative to the detonation wave is equal to the equilibrium sonic speed (2) in the reacted gas behind the wave. These conditions can be calculated more readily than those for a frozen speed of sound for which the ratio of the specific heats k must be calculated (3).

Method of Calculation

Assuming that only the neutral species of H₂O, H₂, O₂, OH, O and H occur in the detonation wave of hydrogen-oxygen mixtures, the Hugoniot equation can be written

$$\frac{p_a}{p_b} = \frac{\left[\frac{(T_a/T_b) \sum_i p_{i,a} (\Delta H_f/RT)_i^{T_a} - (\Delta H_f/RT)_{H_2}^{T_b} + (N_O/N_H)(\Delta H_f/RT)_{O_2}^{T_b}}{2p_{H_2O} + 2p_{H_2} + p_{OH} + p_H} \right] + 1}{\frac{1 + N_O/N_H}{4} \left\{ 1 + \frac{[2p_b/(1 + N_O/N_H)] \cdot (T_a/T_b)}{2p_{H_2O} + 2p_{H_2} + p_{OH} + p_H} \right\}} \quad [1]$$

where

$$\sum p_{i,a} (\Delta H_f/RT)_i^{T_a} = p_{H_2O} (\Delta H_f/RT)_{H_2O}^{T_a} + \dots$$

In Equation [1] the partial pressures of H₂O, H₂, O₂, OH, O and H must satisfy the conditions for chemical equilibrium. With an assumed value for the partial pressure of molecular oxygen, the partial pressures are calculated as

$$p_{O_2} \text{ assumed} \quad p_O = K_{O_2} (p_{O_2})^{1/2} \quad [2]$$

$$p_{H_2} = \left\{ \left[\frac{K_{OH} \left(1 - \frac{N_O}{N_H} \right) (p_{O_2})^{1/2} - \frac{N_O}{N_H} K_{H_2}}{2 \left[\frac{(1 - 2N_O/N_H)(p_{O_2})^{1/2}}{K_{H_2O}} - 2 \frac{N_O}{N_H} \right]} \right]^2 - \frac{2p_{O_2} + K_{O_2} (p_{O_2})^{1/2}}{K_{H_2O} - 2 \frac{N_O}{N_H}} \right\}^{1/2}$$

$$\frac{K_{OH} \left(1 - \frac{N_O}{N_H} \right) (p_{O_2})^{1/2} - \frac{N_O}{N_H} K_{H_2}}{2 \left[\frac{(1 - 2N_O/N_H)(p_{O_2})^{1/2}}{K_{H_2O}} - 2 \frac{N_O}{N_H} \right]} \quad [3]$$

$$p_H = K_{H_2} (p_{H_2})^{1/2} \quad [4]$$

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³ Numbers in parentheses indicate References at end of paper.

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$$p_{OH} = K_{OH} (p_{H_2})^{1/2} \cdot (p_{O_2})^{1/2} \quad [6]$$

$$p_{H_2O} = p_{H_2} (p_{O_2})^{1/2} / K_{H_2O} \quad [6]$$

For hydrogen-rich mixtures ($N_O/N_H < 1/2$) the assumed value of the molecular oxygen partial pressure must be less than $\{2N_O/(N_H - 2N_O)\} \cdot K_{H_2O}^2$.

Since the sum of all partial pressures must be equal to p_a as derived from Equation [1], the correct value of p_{O_2} can be determined by trial and error using Equations [1 through 6]. As a result of these calculations, a pair of T_a and p_a values is obtained that satisfies the Hugoniot equation.

The values of T_a and p_a together with the corresponding partial pressures are then used to calculate the Mach number for the wave relative to the unreacted gas

$$k_b M^2 = \frac{(p_a/p_b) - 1}{1 - \frac{2p_b}{1 + N_O/N_H} \cdot \frac{T_a/T_b}{2p_{H_2O} + 2p_{H_2} + p_{OH} + p_H}} \quad [7]$$

This procedure is repeated until a pair of p_a and T_a values is found which makes this Mach number a minimum. These values and the minimum value of M represent the detonation conditions of a stable Chapman-Jouguet detonation wave. The velocity of the reacted gas relative to the wave is obtained using the continuity equation

$$u_a = u_D \cdot \frac{v_a}{v_b} = u_D \frac{2p_b}{1 + N_O/N_H}$$

$$\frac{T_a/T_b}{2p_{H_2O} + 2p_{H_2} + p_{OH} + p_H} \quad [8]$$

where

$$u_D = [(RT_b/\mathfrak{M}_b) \cdot k_b M_{min}^2]^{1/2}$$

$$M_{min} = M_D$$

The impact pressure ratio follows from

$$\frac{p_{imp}}{p_b} = \frac{(u_D - u_a)^2}{p_b \cdot v_a} + \frac{p_a - p_b}{p_b} = \left[\frac{p_a}{p_b} - 1 \right] \cdot \left[\frac{2p_{H_2O} + 2p_{H_2} + p_{OH} + p_H}{T_a/T_b} \cdot \frac{1 + N_O/N_H}{2p_b} \right] \quad [9]$$

The results of these calculations are presented in Tables 1 through 5. A small amount of scatter in the results was unavoidable because of the limited number of iterations used during these calculations, which were made with a Square Root Friden calculating machine.

Assuming that the immediate front of the detonation wave consists of a normal shock wave, propagating at the velocity u_D through the combustible gas mixture without causing any chemical reactions in the gas, we can calculate the temperature and pressure behind this wave by solving the

Table 1 Composition of combustion gas^a

Molar per cent fuel in mixture	p_b , atm	p_{O_2} , atm	p_O , atm	p_{H_2} , atm	p_H , atm	p_{OH} , atm	p_{H_2O} , atm	p_a, D , atm
30	1	8.724624	0.215919	0.041257	0.020413	0.979947	4.397839	14.38
	5	45.54562	0.720766	0.139228	0.052724	4.272417	23.26924	74.00
	25	234.3475	2.173795	0.425371	0.119158	17.42348	121.5107	376.0
45	100	958.5706	5.325256	1.051486	0.222619	56.44056	502.3895	1524
	1	5.59712	0.764398	0.361456	0.230445	2.640986	7.055621	16.70
	5	29.73052	3.023995	1.450444	0.751872	13.09236	38.15074	86.20
55	25	158.4731	11.10064	5.408457	2.207236	60.89125	206.8194	444.9
	100	690.0791	33.49343	16.46756	5.372824	229.4414	910.1455	1885
	1	2.959380	0.982713	1.038860	0.653540	3.502681	8.362823	17.50
66.67	5	15.83605	4.051083	4.462804	2.283650	17.71854	46.74787	91.10
	25	84.45476	16.17427	18.46938	7.615351	87.57169	259.0146	473.3
	100	364.8844	50.79208	59.26096	19.79955	339.6077	1148.655	1983
66.67 ^b	1	0.745876	0.638231	2.952802	1.390335	3.036375	9.236365	18.00
	5	3.457926	2.651718	14.53298	5.581083	15.41088	50.86544	92.5
	25	16.20487	10.66765	71.40139	21.67408	78.30594	291.7461	490.0
75	100	61.59676	35.43535	279.3280	69.52653	316.8585	1307.255	2070
	1	0.483911	0.435817	1.867628	0.952529	1.915126	5.544988	11.20
	5	2.277220	1.866690	9.424538	3.954084	9.940380	30.83709	58.30
85	25	11.36679	8.142093	49.09055	16.52124	53.89335	184.28593	323.3
	100	41.66044	25.67596	188.1448	50.79253	211.5335	822.1927	1340
	1	0.115846	0.208676	5.607926	1.618600	1.621170	8.327770	17.50
90	5	0.433543	0.749963	29.49570	6.490038	7.612434	45.71833	90.5
	25	1.470763	2.443691	159.1462	25.26848	34.33146	257.3394	480.0
	100	3.720694	5.865815	664.8134	74.87667	115.8869	1134.837	2000
95	1	0.001155	0.005833	9.583973	0.670734	0.191782	5.153881	15.61
	5	0.002658	0.013401	50.28687	2.234858	0.689028	27.13284	80.36
	25	0.004809	0.024271	260.7106	6.655522	2.188263	141.1835	410.77
100	100	0.006513	0.032814	1052.562	15.31090	5.192902	571.6204	1645
	1	0.000005	0.000049	10.01964	0.104141	0.010547	2.865618	13.0
	5	0.000007	0.000066	50.71035	0.268537	0.028007	14.49302	65.5
100	25	0.000008	0.000074	252.2448	0.623218	0.065482	72.06635	325.0
	100	0.000009	0.000084	1025.286	1.340041	0.141945	293.2318	1320

^a Initial temperature = 313.16 K except where noted.

^b Initial temperature = 473.16 K.

Table 2 Properties of a hydrogen-oxygen detonation wave, $p_b = 1$ atm

Molar per cent fuel in mixture	T_b , K	$T_{a, D}$, K	$T_{a, N.S.}$, K	$p_{a, D}$, atm	$p_{a, N.S.}$, atm	p_{imp} , atm	u_a , m/sec	u_D , m/sec	$\frac{\rho_{a, D}}{\rho_b}$	$M_D = \frac{u_D}{a_b}$
30	313.16	2860	1560	14.38	24.174	24.096	1024	1845	1.801	4.567
45	313.16	3320	1795	16.70	28.660	29.296	1169	2182	1.866	4.970
55	313.16	3538	1875	17.50	31.377	30.459	1332	2459	1.846	5.199
66.67	313.16	3646	1981	18.00	32.270	31.572	1522	2826	1.857	5.272
66.67	473.16	3576	2083	11.20	20.666	17.290	1585	2784	1.757	4.225
75	313.16	3567	1976	17.50	32.036	29.917	1750	3173	1.813	5.253
85	313.16	3108	1725	15.61	27.251	26.260	2017	3627	1.798	4.848
90	313.16	2563	1512	13.00	23.215	21.140	2155	3796	1.762	4.476

Table 3 Properties of a hydrogen-oxygen detonation wave, $p_b = 5$ atm

Molar per cent fuel in mixture	T_b , K	$T_{a, D}$, K	$T_{a, N.S.}$, K	$p_{a, D}$, atm	$p_{a, N.S.}$, atm	p_{imp} , atm	u_a , m/sec	u_D , m/sec	$\frac{\rho_{a, D}}{\rho_b}$	$M_D = \frac{u_D}{a_b}$
30	313.16	2965	1586	74.00	122.96	124.32	1033	1861	1.802	4.606
45	313.16	3526	1874	86.20	151.12	149.14	1220	2240	1.836	5.103
55	313.16	3790	2018	91.10	164.37	158.34	1368	2517	1.839	5.321
66.67	313.16	3954	2102	92.50	172.10	157.76	1618	2918	1.803	5.444
66.67	473.16	3884	2182	58.30	109.78	92.586	1652	2869	1.737	4.354
75	313.16	3843	2066	90.50	169.13	152.79	1824	3260	1.787	5.397
85	313.16	3244	1777	80.36	141.26	135.17	2058	3692	1.794	4.935
90	313.16	2596	1525	65.50	117.64	106.19	2177	3821	1.743	4.506

Table 4 Properties of a hydrogen-oxygen detonation wave, $p_b = 25$ atm

Molar per cent fuel in mixture	T_b , K	$T_{a, D}$, K	$T_{a, N.S.}$, K	$p_{a, D}$, atm	$p_{a, N.S.}$, atm	p_{imp} , atm	u_a , m/sec	u_D , m/sec	$\frac{\rho_{a, D}}{\rho_b}$	$M_D = \frac{u_D}{a_b}$
30	313.16	3049	1635	376.0	639.77	628.09	1061	1898	1.789	4.698
45	313.16	3724	1947	444.9	789.00	764.66	1257	2289	1.821	5.214
55	313.16	4064	2104	473.3	865.92	816.96	1417	2583	1.822	5.461
66.67	313.16	4296	2210	490.0	914.05	839.02	1667	3007	1.804	5.610
66.67	473.16	4241	2306	323.3	588.47	535.57	1653	2970	1.796	4.507
75	313.16	4138	2167	480.0	891.60	819.53	1858	3347	1.801	5.541
85	313.16	3349	1816	410.8	725.31	689.79	2092	3741	1.788	5.001
90	313.16	2606	1535	325.0	592.15	520.75	2209	3834	1.736	4.521

Table 5 Properties of a hydrogen-oxygen detonation wave, $p_b = 100$ atm

Molar per cent fuel in mixture	T_b , K	$T_{a, D}$, K	$T_{a, N.S.}$, K	$p_{a, D}$, atm	$p_{a, N.S.}$, atm	p_{imp} , atm	u_a , m/sec	u_D , m/sec	$\frac{\rho_{a, D}}{\rho_b}$	$M_D = \frac{u_D}{a_b}$
30	313.16	3108	1663	1524	2603.2	2543.2	1072	1914	1.786	4.738
45	313.16	3898	2004	1885	3265.2	3327.0	1248	2328	1.864	5.303
55	313.16	4298	2227	1983	3685.0	3395.1	1477	2664	1.803	5.632
66.67	313.16	4641	2296	2070	3819.0	3597.2	1683	3073	1.826	5.733
66.67	473.16	4554	2387	1340	2448.5	2236.3	1674	3019	1.803	4.581
75	313.16	4380	2231	2000	3710.1	3431.2	1890	3413	1.806	5.651
85	313.16	3405	1840	1645	2945.5	2731.8	2132	3770	1.769	5.039
90	313.16	2622	1539	1320	2375.1	2139.7	2189	3839	1.755	4.527

following equations simultaneously

$$\frac{p_{a, N.S.}}{p_b} = \frac{1}{2} + \sum_i \gamma_i' \left[\left(\frac{H - E_0}{RT} \right)_i^{T_{a, N.S.}} \cdot \frac{T_{a, N.S.}}{T_b} - \left(\frac{H - E_0}{RT} \right)_i^{T_b} \right] - \frac{1}{2} \frac{T_{a, N.S.}}{T_b} + \left(\frac{1}{2} + \sum_i \gamma_i' \times \right. \\ \left. \left[\left(\frac{H - E_0}{RT} \right)_i^{T_{a, N.S.}} \cdot \frac{T_{a, N.S.}}{T_b} - \left(\frac{H - E_0}{RT} \right)_i^{T_b} \right] - \frac{1}{2} \frac{T_{a, N.S.}}{T_b} \right)^2 + \frac{T_{a, N.S.}}{T_b} \right)^{1/2} \quad [10]$$

$$\frac{p_{a, N.S.}}{p_b} = \frac{1 + k_b M_D^2}{2} + \left[\left(\frac{1 + k_b M_D^2}{2} \right)^2 - \frac{T_{a, N.S.}}{T_b} \cdot k_b M_D^2 \right]^{1/2} \quad [11]$$

These pressures are the highest that would occur in the detonation wave should complete relaxation prevail in the internal modes of motion of the unreacted gases. Completely inactive vibrational motion in the molecules of the combustible gas mixtures would lead to pressures and temperatures in the wave calculated for a normal shock at M_D with

$$[(H - E_0)/RT]^{T_a} = [(H - E_0)/RT]^{T_b}$$

The difference between the latter values and those obtained from Equations [10 and 11] is usually quite small.

It is frequently necessary to calculate the parameters behind a steady-state detonation wave for the case where the reaction has proceeded to an arbitrarily assumed chemical composition. For such calculations a method is proposed which is based on an evaluation of the derivative $d(p_a/p_b)/d(T_a/T_b)$ which, according to the Chapman-Jouguet condition

$$\frac{d \left(\frac{u_D^2}{RT_b/\mathfrak{M}_b} \right)}{d \left(\frac{T_a}{T_b} \right)} = \left\langle \left(1 - \frac{T_a}{T_b} \cdot \frac{\mathfrak{M}_a}{\mathfrak{M}_b} \right) \cdot \frac{d \left(\frac{p_a}{p_b} \right)}{d \left(\frac{T_a}{T_b} \right)} - \left(\frac{p_a}{p_b} - 1 \right) \left[\frac{T_a}{T_b} \cdot \frac{\mathfrak{M}_a}{\mathfrak{M}_b} \frac{d(p_a/p_b)}{d(T_a/T_b)} - \frac{p_a}{p_b} \cdot \frac{\mathfrak{M}_a}{\mathfrak{M}_b} \right] \right\rangle \div \left\langle \left(1 - \frac{T_a}{T_b} \cdot \frac{\mathfrak{M}_a}{\mathfrak{M}_b} \right)^2 \right\rangle = 0 \quad [12]$$

becomes

$$\frac{d \left(\frac{p_a}{p_b} \right)}{d \left(\frac{T_a}{T_b} \right)} = - \frac{\frac{p_a}{p_b} - 1}{\frac{p_a}{p_b} \cdot \frac{\mathfrak{M}_a}{\mathfrak{M}_b} - \frac{T_a}{T_b} \left[2 - \frac{1}{(p_a/p_b)} \right]} \quad [13]$$

Upon differentiation of the Hugoniot equation

$$\frac{p_a}{p_b} = \frac{T_a/T_b}{\mathfrak{M}_a/\mathfrak{M}_b} \left[\sum_i \gamma_i'' \left(\frac{\Delta H_f}{RT} \right)_i^{T_a} - \frac{1}{2} \right] - \left[\sum_i \gamma_i' \left(\frac{\Delta H_f}{RT} \right)_i^{T_b} - \frac{1}{2} \right] + \left(\frac{T_a/T_b}{\mathfrak{M}_a/\mathfrak{M}_b} \left[\sum_i \gamma_i'' \left(\frac{\Delta H_f}{RT} \right)_i^{T_a} - \frac{1}{2} \right] - \left[\sum_i \gamma_i' \left(\frac{\Delta H_f}{RT} \right)_i^{T_b} - \frac{1}{2} \right] \right)^2 + \frac{T_a/T_b}{\mathfrak{M}_a/\mathfrak{M}_b} \right)^{1/2} \quad [14]$$

this derivative becomes

$$\frac{d(p_a/p_b)}{d(T_a/T_b)} = \frac{\sum_i \gamma_i'' (c_p/R)_i^{T_a} - 1/2}{\mathfrak{M}_a/\mathfrak{M}_b} + \left\langle \frac{T_a/T_b}{\mathfrak{M}_a/\mathfrak{M}_b} \left[\sum_i \gamma_i'' \left(\frac{\Delta H_f}{RT} \right)_i^{T_a} - \frac{1}{2} \right] - \left[\sum_i \gamma_i' \left(\frac{\Delta H_f}{RT} \right)_i^{T_b} - \frac{1}{2} \right] \right\rangle \div \left\langle \left(\frac{T_a/T_b}{\mathfrak{M}_a/\mathfrak{M}_b} \left[\sum_i \gamma_i'' \left(\frac{\Delta H_f}{RT} \right)_i^{T_a} - \frac{1}{2} \right] - \left[\sum_i \gamma_i' \left(\frac{\Delta H_f}{RT} \right)_i^{T_b} - \frac{1}{2} \right] \right)^2 + \frac{T_a/T_b}{\mathfrak{M}_a/\mathfrak{M}_b} \right\rangle^{1/2} \quad [15]$$

The detonation parameters are obtained by solving Equations [13, 14 and 15] simultaneously.

An approximate but explicit solution of the detonation problem is possible when an average value for the specific heat ratio k is introduced. According to this method, the detonation wave is considered to consist of a shock wave followed by a region in which heat is added to the gas until the Mach number becomes 1. This solution is useful primarily because it yields a quick answer, and it affords a good starting point for the exact calculations. When heat q is

added to a unit mass of the subsonic flow behind the normal shock, the final Mach number M_3 will be 1 if, for a given value of q , the proper value of M_1 is selected. The amount of heat q added to the gas is the heat of reaction of a unit mass of the gas mixture. Allowance must be made for the fact that the reaction does not go to completion in most cases. Since for the normal shock M_2^* equals $1/M_1^*$, and for the flow with heat addition in the present case M_3 equals M_3^* equals 1 which leads to

$$\frac{[1 - (M_2^*)^2]^2}{4(M_2^*)^2} = \frac{q}{h_1 + \frac{u_1^2}{2}} = \frac{\frac{q}{(\mathfrak{R}T_1/\mathfrak{M}_1)}}{\frac{k}{k-1} \left(1 + \frac{k-1}{2} M_1^2 \right)} \quad [16]$$

we obtain

$$M_1^2 = \frac{k^2 - 1}{k} \frac{q}{(\mathfrak{R}T_1/\mathfrak{M}_1)} + 1 + \left[\left(\frac{k^2 - 1}{k} \frac{q}{(\mathfrak{R}T_1/\mathfrak{M}_1)} \right)^2 - 1 \right]^{1/2} \quad [17]$$

for the Mach number of the detonation wave. Results of these calculations are presented in Figs. 1 and 2 for various values of the specific heat ratio k as a function of the heat release coefficient

$$C_q = q/(\mathfrak{R}T_1/\mathfrak{M}_1)$$

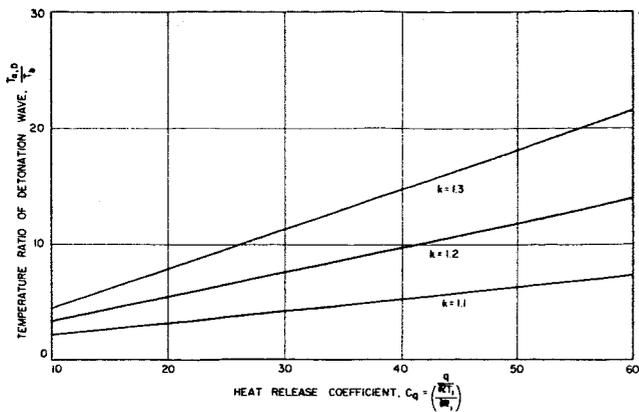


Fig. 1 Effect of heat release coefficient on temperature ratio across detonation wave for hydrogen-oxygen mixtures

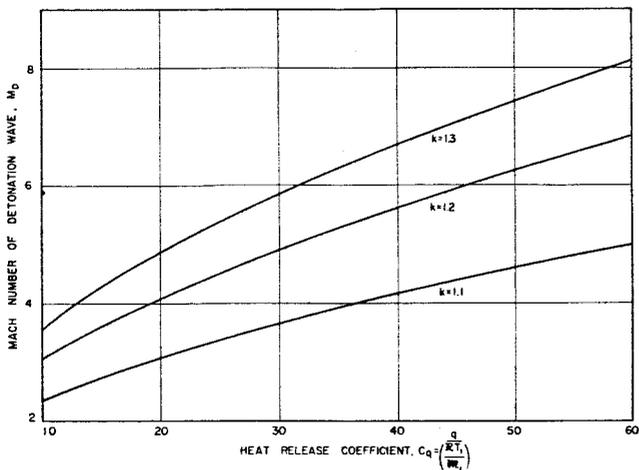


Fig. 2 Effect of heat release coefficient on Mach number of detonation wave for hydrogen-oxygen mixtures

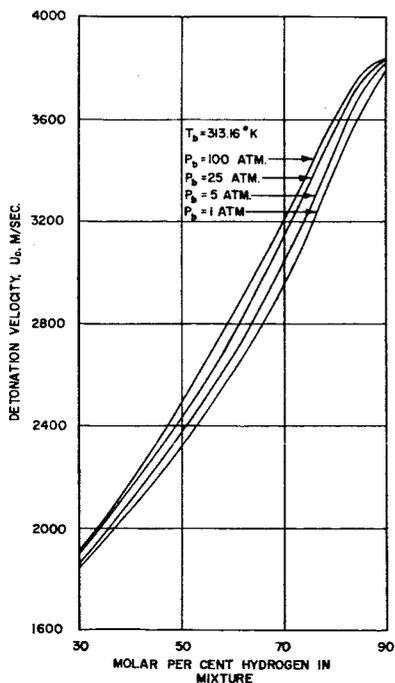


Fig. 3 Calculated detonation velocity of hydrogen-oxygen mixtures as a function of fuel concentration

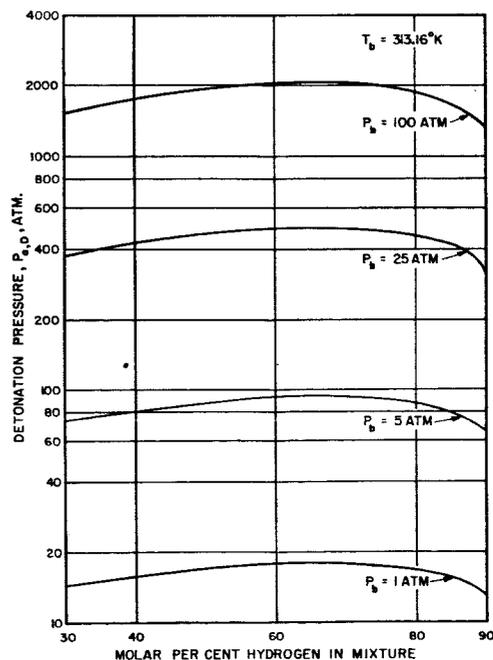


Fig. 4 Pressure behind hydrogen-oxygen detonation wave for various fuel concentrations

Discussion of Results

The results of the calculations show that the detonation velocities of stoichiometric hydrogen-oxygen mixtures (Fig. 3) increase with initial pressure at the approximate rate of $d(u_D)/(dp/p) = 54$ m per sec. This coefficient becomes smaller for lean or rich mixtures. The curves of Fig. 3 also show that the detonation velocities of hydrogen-oxygen mixtures increase rather sharply with the concentration of hydrogen in mixtures up to 90 per cent. At higher hydrogen concentrations the advent of a decrease in velocity is indicated by the shape of the curves.

The pressure ratio $p_{s,D}/p_0$ across the detonation wave of near stoichiometric mixtures increases rather significantly when the initial pressure is increased (Fig. 4). For very lean or very rich mixtures the effect is small. The temperature of the gas behind the detonation wave follows a similar pattern (Fig. 5). However, the density ratio $\rho_{s,D}/\rho_0$ across the wave decreases as the initial pressure is increased. For lean or rich mixtures, again, the effect of pressure on this parameter is small.

Variations of the initial temperature have only a small influence on the detonation velocity, the detonation temperature and the density ratio across the wave. However, these variations affect the pressure in the wave very strongly. Whereas an increase of 160 C (50 per cent) in the initial temperature produces a decrease of the detonation velocity by less than 2 per cent, this temperature change decreases the pressure by more than 30 per cent. It is of interest to note that an increase in initial temperature leads to a lower detonation temperature.

The temperatures in the normal shock zone are almost one half the detonation temperatures, whereas the pressures behind the normal shock are almost twice the pressure of the detonation wave and slightly higher than the impact pressures.

The results of these theoretical calculations are being used in an experimental investigation to determine the detonation induction distances of hydrogen-oxygen mixtures under a variety of initial conditions. Velocity measurements and other pertinent data obtained during this experimental study will be presented later.

Acknowledgment

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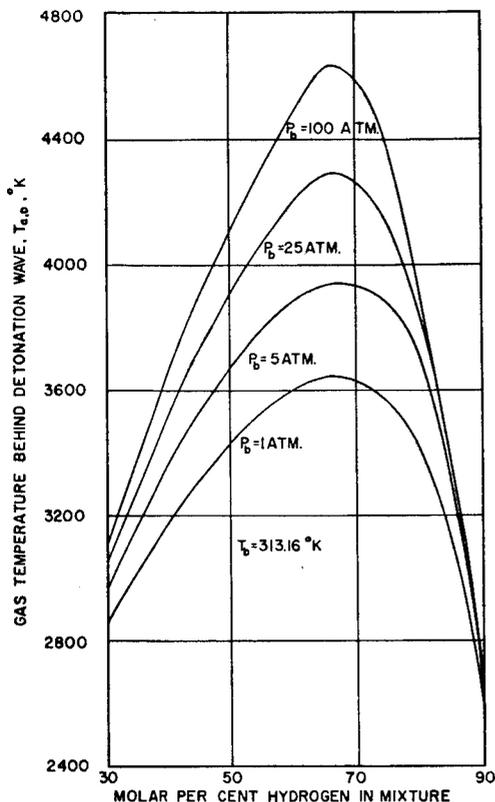


Fig. 5 Gas temperature behind hydrogen-oxygen detonation wave as a function of fuel concentration for various initial pressures

Nomenclature

a	= equilibrium sonic velocity in gas mixture
c_p	= specific heat at constant pressure
C_q	= heat release coefficient
E_0	= zero point energy
H	= absolute molar enthalpy
$\left(\frac{\Delta H_f}{RT}\right)_i$	= dimensionless heat of formation of species i at temperature T
k	= ratio of specific heat at constant pressure to that at constant volume
K	= equilibrium constant based on partial pressures
M	= Mach number
\mathcal{M}	= molecular weight
N	= total mole number of element in mixture
p	= absolute pressure
p_i	= partial pressure of species i
q	= heat added per unit mass of gas
R	= universal gas constant
s	= entropy per unit mass
T	= absolute temperature
u	= linear velocity
v	= specific volume
γ_i'	= mole fraction of reactants
γ_i''	= mole fraction of products
ρ	= density

Subscripts

a	= conditions in gas leaving detonation or shock wave
b	= conditions in gas entering detonation or shock wave
D	= stable detonation wave
i	= i th species of mixture
imp	= impact
min	= minimum
N.S.	= normal shock wave
1	= initial state of gas
2	= state of gas behind normal shock when initial Mach number is M_1
3	= state of gas behind steady-state detonation wave
*	= critical flow condition

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